**Project Diary**

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**Programme:** Molecular Technique in Life Science

**Course:** Project in molecular Life science (KB8024/KB8025)

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| **Date** | **Work** |
| Feb 15th, 2018 | 1) Read *Noble WS (2009) A Quick Guide to Organizing Computational Biology Projects. PLOS Computational Biology 5(7): e1000424.* [*https://doi.org/10.1371/journal.pcbi.1000424*](https://doi.org/10.1371/journal.pcbi.1000424)  2) Read [Linux Tips and Tricks](http://bioinfo.se/courses/project-in-molecular-life-science-kb7006/lessons/linux-tips-and-trix/) + [How to organize your project](http://bioinfo.se/courses/project-in-molecular-life-science-kb7006/lessons/organize-project/)  3) Created GitHub account |
| Feb 16th | 1) Practice Bash Command: <http://swcarpentry.github.io/shell-novice/>  2) Practice Git Command: <http://swcarpentry.github.io/git-novice> |
| Feb 17th | 1) Practiced Bash Command, Write bash scripts  2) Start literature search about “Protein secretion”, “Signal peptide”, and “Gram-negative bacteria” |
| Feb 18th | Literature review |
| Feb 19th, 2018 | 1) Reorganized folders on GitHub  2) Finished week1 assignment: createfolder.sh <https://github.com/YouchengZHANG/project/tree/master/assignment/week1> |
| Feb 20th | 1) Add Project Diary  2) Start literature search about “Signal peptide prediction”, “Machine learning approaches”, “Neural network method” and “Random Forest”  3) Start week2 assignment: Summary of 5 relevant papers  4) Finished Python Command: <http://swcarpentry.github.io/python-novice-inflammation/> |
| Feb 21st | 1) Write and Add week2 assignment: List\_of\_papers\_and\_Summary.pdf  <https://github.com/YouchengZHANG/project/tree/master/assignment/week2>  2) Read *Costa, T. R. et al. Secretion systems in Gram-negative bacteria: structural and mechanistic insights. Nature reviews. Microbiology* ***13****, 343-359, doi: 10.1038/nrmicro3456 (2015).*  3) Read *Chou, K. C. Prediction of protein signal sequences. Current protein & peptide science* ***3****, 615-622 (2002).*  4) Write week2 assignment: Project\_plan |
| Feb 22nd | 1) Read *Zeiler, M.D. and Fergus, R., 2014, September. Visualizing and understanding convolutional networks. In European conference on computer vision (pp. 818-833). Springer, Cham*.  2) Learn sklearn and one-hot encoding  3) Extract feature using part of the raw data |
| Feb 23rd | 1) Journal Club and Learn convolutional networks  2) Learn sklearn.svm and cross-validation |
| Feb 24th | 1) Write Feature Extractor  2) Run SVM with different kernel and parameters and Run different cross-validation  3) Write Window size operator  4) Learn how to save and load the trained model |
| Feb 25th | 1) Read and Learn how to process PSSM *Jones, D.T., 1999. Protein secondary structure prediction based on position-specific scoring matrices1. Journal of molecular biology, 292(2), pp.195-202*.  2) Read literatures about “PSSM normalization from raw profile matrix value” and “scaling window size in signal peptide prediction”:  *Sharma, R., Sharma, A. et al. 2015. Predict gram-positive and gram-negative subcellular localization via incorporating evolutionary information and physicochemical features into Chou's general PseAAC. IEEE transactions on nanobioscience, 14(8), pp.915-926.*  *Chou, K.C., 2001. Prediction of signal peptides using scaled window. peptides, 22(12), pp.1973-1979.*  3) Try to write both bash and python scripts for separating each sequence information into single files and then running PSI-BLAST locally  4) Learn additional Bash Command: variable assignment, calculation, input/output, $ sed/awk  5) Learn how to manage background jobs: $ &, $ nohup, $ screen  6) Write PSSM extractor |
| Feb 26th , 2018 | 1) Test PSI-BLAST locally, change parameter e.g. -num\_thread, -word\_size to estimate running time  2) Learn background command: $ jobs, $ ps -aux, $ kill, $ lscpu, $ top -H  2) Write PSSM window size operator  3) Modify the window size parameter from [(i – n)…i…(i + n)] to [(i – m)…i…(i + n)] where the two edges of window size could be different |
| Feb 27th | 1) Test PSI-BLAST with uniref90, uniref50 and swissprot database, as well as with different evalue  2) Run SVM on various number of samples in raw dataset to evaluate and estimate the running time  3) Look for solutions to speed up the training process |
| Feb 28th | 1) Modify the Feature Extractor without using OneHotEncoder() command  2) Modify the Feature Extractor to a user-friendly program  3) Run PSI-BLAST on the raw dataset (9357 sequences) and Get the .align / .pssm files  4) Test the PSSM editor and extractor  5) Learn different classifiers in sklearn: RandomForestClassifier; OneVsRestClassifier; BaggingClassifier, etc.  6) Practice presentation |
| Mar 1st |  |
| Mar 2nd |  |
| Mar 3rd |  |
| Mar 4th |  |
| Mar 5th , 2018 |  |
| Mar 6th |  |
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